

The Asymptotic Cooling of Heat-Bath Algorithmic Cooling

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The purity of quantum states is a key requirement for many quantum applications. Improving the purity is limited by fundamental laws of thermodynamics. Here we are probing the fundamental limits for a natural approach to this problem, namely heat-bath algorithmic cooling (HBAC). The existence of the cooling limit for HBAC techniques was proved by Schulman et al., the limit however remained unknown for the past decade. Here for the first time we establish this limit. In the context of quantum thermodynamics, this corresponds to the maximum extractable work from the quantum system. We also establish, in the case of higher dimensional reset systems, how the performance of HBAC depends on the energy spectrum of the reset system.

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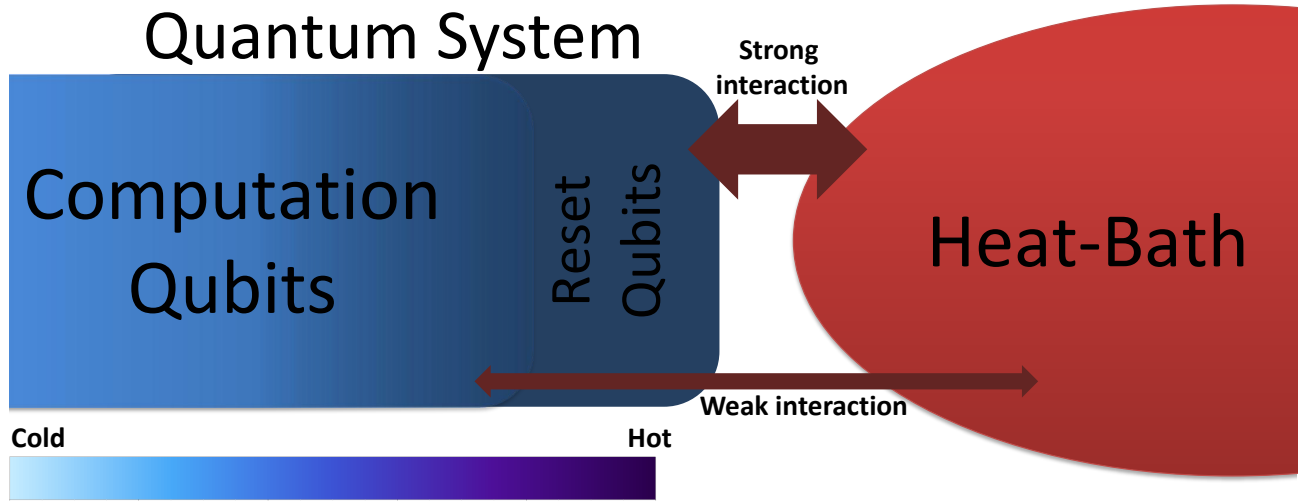


Figure 1. The schematic of the model. The quantum system comprises computation qubits and reset qubits and interacts with a heat-bath. The heat-bath incorporates degrees of freedom in the environment that couple to the qubits in the quantum system. Usually, different qubits couple differently to these degrees of freedom. The computation qubits interact weakly and the reset qubits interact strongly with the heat-bath. We ignore the weak interaction between the computation qubits and the heat-bath and assume that only the reset qubits are effected by the interaction with the heat-bath. The goal is to cool down the qubits in the system. Note that this is just a schematic and in reality they are not necessarily spatially arranged in this way. The HBAC does not cool all the qubits to the same temperature and the asymptotic temperature of different computation qubits would be different. We find the asymptotic state and consequently the temperature for all the qubits including the first one which is the cooling limit for all the HBAC techniques.

The purity of quantum states is often one of the limiting factors in many applications and quantum technologies. For instance, the signal to noise ratio (SNR) in spectroscopy and medical imaging [1–5] or the resolution in metrology and quantum sensing [6–9] are often limited by the purity of the quantum states. High purity is also a necessity for quantum computation. Fault-tolerant quantum computing relies on using fresh ancillary quantum bits. Recently Ben-Or, Gottesman and Hassidim proposed a quantum refrigerator to prepare high purity quantum states for this purpose using algorithmic cooling [10].

Different methods have been exploited to improve the purity but all of these techniques are limited by the laws of thermodynamics [11, 12]. It is interesting both fundamentally and practically to understand these limits. In the context of quantum thermodynamics, extracting work from a quantum system is equivalent to increasing its purity and cooling it [13] and cooling limits correspond to Carnot-like efficiency limits. Quantum thermodynamics has been studied as a resource theory of purity [13–15] and recently Horodecki and Oppenheim extended this paradigm for general thermodynamic transformations. They found the limit for the extractable work in terms of relative entropy when the Hamiltonian of the process is time independent. Usually quantum applications involve quantum control which means that the Hamiltonian is time-dependent, and in these cases their result gives an upper bound.

Heat-bath algorithmic cooling is another method which takes a more practical approach to the cooling problem. Here a natural subclass of general thermodynamic transformations is considered where we have control over a part of the system, and have limited control over how the system interacts with an external heat-bath [12, 16]. This model applies to a wide range of quantum implementation techniques like nuclear magnetic resonance (NMR) [17–19], ion-traps [20] and recently in quantum optics [21]. The HBAC methods have also been studied from the thermodynamic viewpoint [16, 22].

Here we consider a quantum system that is in interaction with a heat-bath. The quantum system comprises two kind of qubits, the computation qubits and the reset qubits. The computation qubits are the high quality qubits with long decoherence time that are used for computation. The reset qubits on the other hand have shorter relaxation time and equilibrate fast. Figure 1 shows a schematic of the model that we are considering in our work.

This model applies to a variety of physical systems. For instance, in NMR, the system is the few nuclear spins that can be controlled and the heat-bath comprises the other magnetic moments in the sample. These magnetic moments couple to the nuclear spins in the system and eventually equilibrate them. Different spin species have different coupling rates [17, 18].

The class of cooling transformations that we are considering here are known as heat-bath algorithmic cooling [18, 23, 24]. HBAC is a quantum computation technique for cooling computation qubits by transferring their entropy

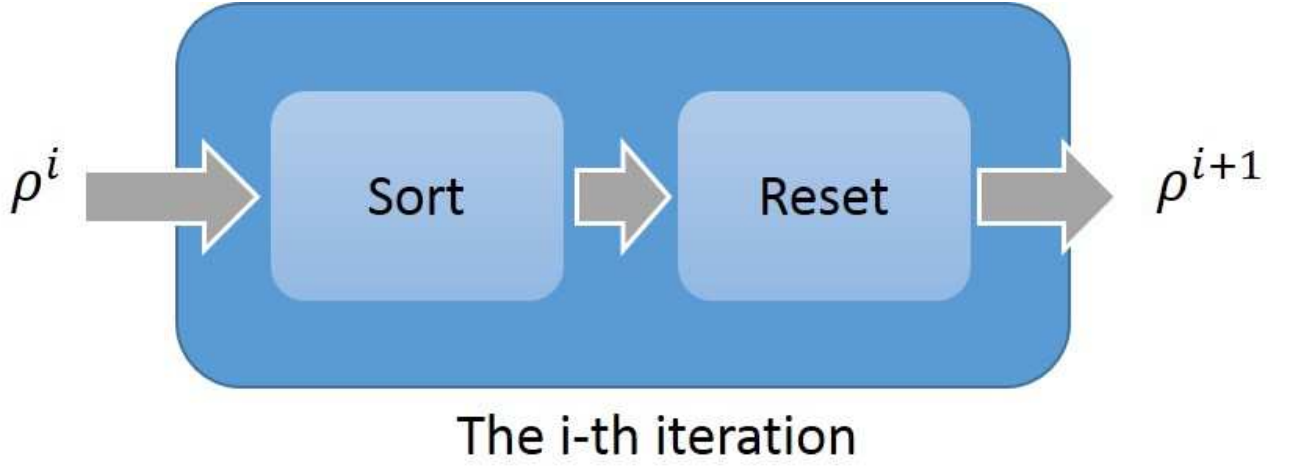


Figure 2. The schematics of each iteration of PPA algorithmic cooling. The diagonal elements of the density matrix are first sorted, which increases the polarization of the first computation qubit and decreases the polarization of the reset qubit. Next the reset process, refreshes the reset qubit and restores its initial polarization.

to the reset qubits. The reset qubits are regularly refreshed through their interaction with the heat-bath.

The original idea of algorithmic cooling was developed by Schulman and Vazirani in [25] which uses a technique for Schumacher’s quantum data compression [26, 27]. Later it was proposed to use a heat-bath to enhance the cooling beyond the compression bounds[23, 28]. The idea is that after the entropy transfer, the heat-bath refreshes the hot qubits and then the entropy transfer can be repeated. Different iterative methods were developed based on this idea[27, 29, 30]. All of these methods are referred to as “Heat-Bath Algorithmic Cooling”.

In [24] Schulman et al. established a lower-bound for the asymptotic temperature and proved that none of these iterative techniques can extract all of the entropy from the computation qubits. However, the asymptotic cooling limit remained unknown. In [29], a steady state of HBAC was identified and was used to establish an upper-bound for the limit under the assumption that HBAC starts from the maximally mixed state and converges to a steady state.

In this work, we show that this process has an asymptotic state and find this asymptotic state of the computation and reset qubits. This gives the cooling limit of the qubits in this framework. This fundamental limit sets the ultimate limit of any practical cooling approach under similar constraints.

We use the technique that was introduced in [24]. It is called the “Partner Pairing Algorithm (PPA)” and is the optimal technique for HBAC. We find the cooling limit for the PPA and as it is the optimal technique, the limit applies to all the HBAC techniques as well.

The PPA is an iterative method. In each iteration, the diagonal elements of the density matrix are sorted and then the reset qubit is refreshed. For example, if we have $n = 1$ computational qubits, plus one reset qubit, with combined probabilities corresponding to 0.45 for $|00\rangle$, 0.15 for $|01\rangle$, 0.3 for $|10\rangle$ and 0.1 for $|11\rangle$, then the sort step will swap $|01\rangle$ and $|10\rangle$. After this swap step, the probabilities of the computational basis states are in decreasing order with respect to the lexicographic ordering of the qubits, which corresponds to increasing the probability of a 0 in the leftmost qubit. The reset process is equivalent to

$$R(\rho) = \text{Tr}_R(\rho) \otimes \rho_R. \quad (1)$$

$\text{Tr}_R(*)$ is the partial trace over the reset qubit and $\rho_R = \frac{1}{e^{-\epsilon} + e^{\epsilon}} \begin{pmatrix} e^{\epsilon} & 0 \\ 0 & e^{-\epsilon} \end{pmatrix}$, is the fixed point of the reset process. The parameter ϵ is called the polarization and $\epsilon = \frac{\Delta}{2K_b T_B}$, where Δ is the energy gap of the reset qubit, K_b is the Boltzmann constant, and T_B is the temperature of the heat-bath. Polarization is commonly used to quantify the purity of spins. The higher the polarization, the purer and colder the qubit is. For a qubit with the state $\rho = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}$ the polarization is given by $\frac{1}{2} \log \left(\frac{a}{b} \right)$.

The reset step cools down the reset qubit and changes the diagonal elements of the density matrix which also changes their ordering. The sort operation in the following iteration would then increase the polarization of computation qubits. Figure 2 shows the procedure of each iteration.

We use $[\rho^t] = \{\lambda_1^{(t)}, \lambda_2^{(t)}, \dots, \lambda_{2^{n+1}}^{(t)}\}$ to show the state of n computation qubits plus one reset qubit which is the last one. The superscript represents the iteration index and the subscript is the index of the diagonal elements.

HBAC cools the first qubit monotonically which means that we just need to find the asymptotic temperature to find the cooling limit. If the system converges to an asymptotic state (which we show happens), then this state determines the cooling limit.

Despite the simplicity of each iteration, the dynamics are complicated and it is difficult to understand how the state evolves under these dynamics. In particular, even assuming the system converges to an asymptotic state, it is challenging to find the asymptotic state [29, 30]. Note that the sort operation depends on the probability distribution and thus is changing in each iteration and as a result, the cooling process is not a time-homogeneous Markov process.

We use the fact that an asymptotic state should be invariant under PPA and first identify steady states of the PPA. This gives a necessary condition for the asymptotic state. We then specify the asymptotic state by proving a condition on the dynamics of PPA.

The asymptotic state does not change under the operations of HBAC and is a fixed point of the dynamics. Technically this implies that if it is reset, it still will be sorted. The state after the reset is $[\rho^\infty] = \{p_0^\infty, p_1^\infty, \dots, p_{2^n-1}^\infty\} \otimes [\rho_R]$, where the first part represents the state of the n computation qubits.

The fact that the full density matrix is sorted after the reset step, implies that $p_i^\infty e^{-\epsilon} \geq p_{i+1}^\infty e^\epsilon, \forall i$.

Note that this condition does not specify the asymptotic state. In fact the steady state is not unique and any state that satisfies the condition above is invariant under PPA. Therefore the invariance under PPA is a necessary condition, but not sufficient. This was also recognized in [29] where the state in Equation (4) was found and shown to establish a lower bound on the asymptotic polarization. Their numerical evidence [29], and other numerical studies independent of this work [31], suggested the bound is tight when the initial state is maximally mixed.

One of the key elements of our work is the following theorem which specifies the steady state that is the asymptotic state of HBAC. It states that while the distances between consecutive p_i are increasing in PPA, the ratio of two consecutive diagonal elements of the density matrix would never exceed $e^{2\epsilon}$.

Theorem 1. *For PPA algorithmic cooling with a reset qubit $[\rho_R] = \frac{1}{e^{-\epsilon} + e^\epsilon} \{e^\epsilon, e^{-\epsilon}\}$, for any iteration t and $i, 0 \leq i \leq 2^n - 1$, $\frac{p_i^t}{p_{i+1}^t} \leq \max \left\{ e^{2\epsilon}, \frac{p_i^0}{p_{i+1}^0} \right\}$.*

The sketch of the proof is as follows. For any index i and any iteration t , if the ratio of $\frac{p_i^t}{p_{i+1}^t} \leq e^{2\epsilon}$, then we can show that $p_i^{t+1} \leq e^\epsilon (p_i^t + p_{i+1}^t)$ and $p_{i+1}^{t+1} \geq e^{-\epsilon} (p_i^t + p_{i+1}^t)$ and as a result $\frac{p_i^{t+1}}{p_{i+1}^{t+1}} \leq e^{2\epsilon}$. On the other hand, if the ratio of $\frac{p_i^t}{p_{i+1}^t} \geq e^{2\epsilon}$, then it is easy to see that $\frac{p_i^{t+1}}{p_{i+1}^{t+1}} \leq \frac{p_i^t}{p_{i+1}^t}$. Note that the sort operation in this case could only decrease p_i or increase p_{i+1} , both of which leads to a lower $\frac{p_i^{t+1}}{p_{i+1}^{t+1}}$. Therefore we can always bound $\frac{p_i^{t+1}}{p_{i+1}^{t+1}} \leq \max \left\{ e^{2\epsilon}, \frac{p_i^t}{p_{i+1}^t} \right\}$. Induction on t completes the proof of the theorem. A more detailed proof is given in the supplementary material.

If the initial state satisfies $d_i^0 \leq 2\epsilon$ for all i , which holds, for a broad class of states like the maximally mixed state or the thermal state when the computation qubits have a smaller gap than the reset qubit, then one obtains the following condition for the asymptotic state:

$$p_i^\infty e^{-\epsilon} = p_{i+1}^\infty e^\epsilon, \forall i, \quad (2)$$

where p_i are the diagonal elements of the density matrix of computation qubits. Note that in general, it could be that $d_i^0 \geq 2\epsilon$. We investigate the more general case in the supplemental materials.

This condition together with the normalization of the state is enough to determine the full state. Equation (2) can be rewritten as $p_i^\infty = e^{-2i\epsilon} p_0^\infty$ and considering state normalization gives:

$$p_0^\infty = \frac{e^{-2\epsilon} - 1}{(e^{-2\epsilon})^{2^n} - 1}. \quad (3)$$

Schulman et al. upper bounded λ_1^∞ by $\frac{e^{2^n \epsilon}}{2^n}$ in [24] which is consistent with our result. Note that $\lambda_1^\infty = \frac{e^\epsilon}{e^{-\epsilon} + e^\epsilon} p_0^\infty$. Figure 3 gives a comparison between this bound and the actual value from equation (3). Plots are for $n = 2$ and one reset qubit. Figure 3 illustrates how the upper bound in [24] gets looser as ϵ increases.

Equations (2) and (3) give the asymptotic state

$$[\rho^\infty] = p_0^\infty \{1, e^{-2\epsilon}, e^{-4i\epsilon}, \dots\} \otimes \rho_R. \quad (4)$$

The first qubit has the lowest temperature. Therefore, we focus on the first computation qubit for finding the cooling limit. We find that the polarization of the first qubit is

$$P = 2^{n-1} \epsilon. \quad (5)$$

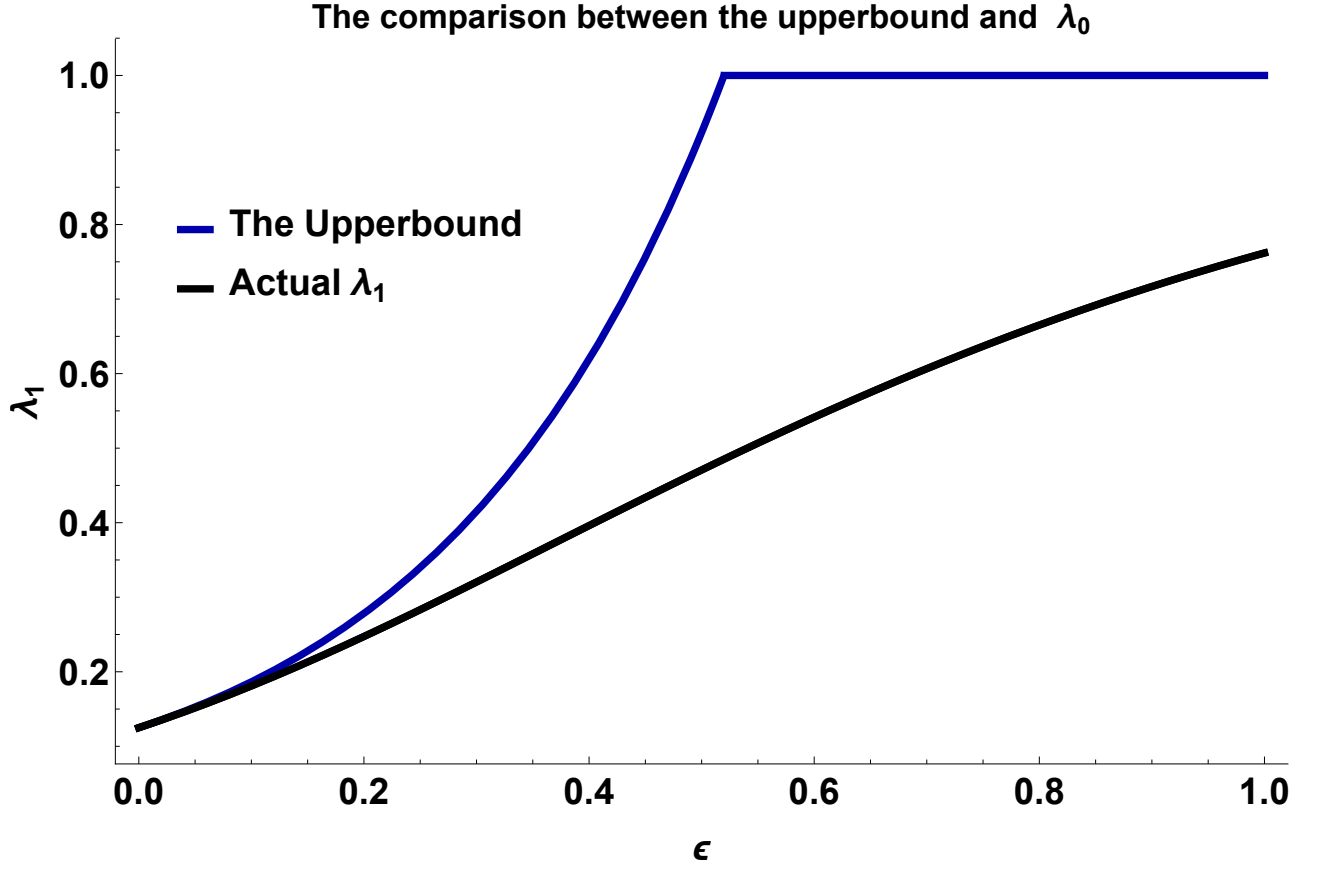


Figure 3. Comparison of the upper bound and value of λ_1^∞ . The gap between the upper bound and the actual value gets larger as ϵ , the polarization of the reset qubit increases. ^a

^a Thanks to N. Rodrigues Briones and R. Laflamme for catching a glitch in an earlier version of this plot.

This result is consistent with the lower bound that was calculated in [29], in the case of $\epsilon \ll \frac{1}{2^n}$. In fact we proved that this lower-bound is tight.

Equation (5) shows that the performance of HBAC increases exponentially with the number of qubits, n . The simple way to see this is to look at the effective temperature. The effective temperature of the first qubit is

$$T_{\text{eff}} = \frac{\delta}{\Delta} \frac{T_B}{2^{n-1}}, \quad (6)$$

where δ is the energy gap of the qubit and is often different from Δ , the energy gap of the reset qubit. Usually the reset and computation qubits should be of different species as the reset qubits have a shorter relaxation time. The cooling limit would improve if the energy gap of the reset qubit is much larger than the one for the computation qubits. For instance, if an electron is used as the reset qubit and hydrogen nuclear spins for computation, this ratio would be $\frac{1}{660}$ which lowers the cooling limit by a factor of 660.

Figure 4 shows how the effective temperature decreases with increasing the number of computation qubits, n . It also shows that changing the $\frac{\delta}{\Delta}$ changes the cooling limit.

We can also answer one of the important questions about HBAC, namely, identifying how the performance of HBAC depends on the energy spectrum of the reset system in the case of higher dimensional reset systems.

Equation (2) can be generalized for arbitrary reset state, ρ_R . For a D -level reset system we get a similar condition as in equation (2) with the difference that the gap is replaced by the sum of the gaps. We refer to this as the “large gap” and use Δ_{total} to show it. The cooling limit for qudits is

$$T_{\text{eff}} = \frac{\delta}{\Delta_{\text{total}}} \frac{T_B}{2^{n-1}}, \quad (7)$$

which similar to the one in Equation (6) with Δ replaced by Δ_{total} .

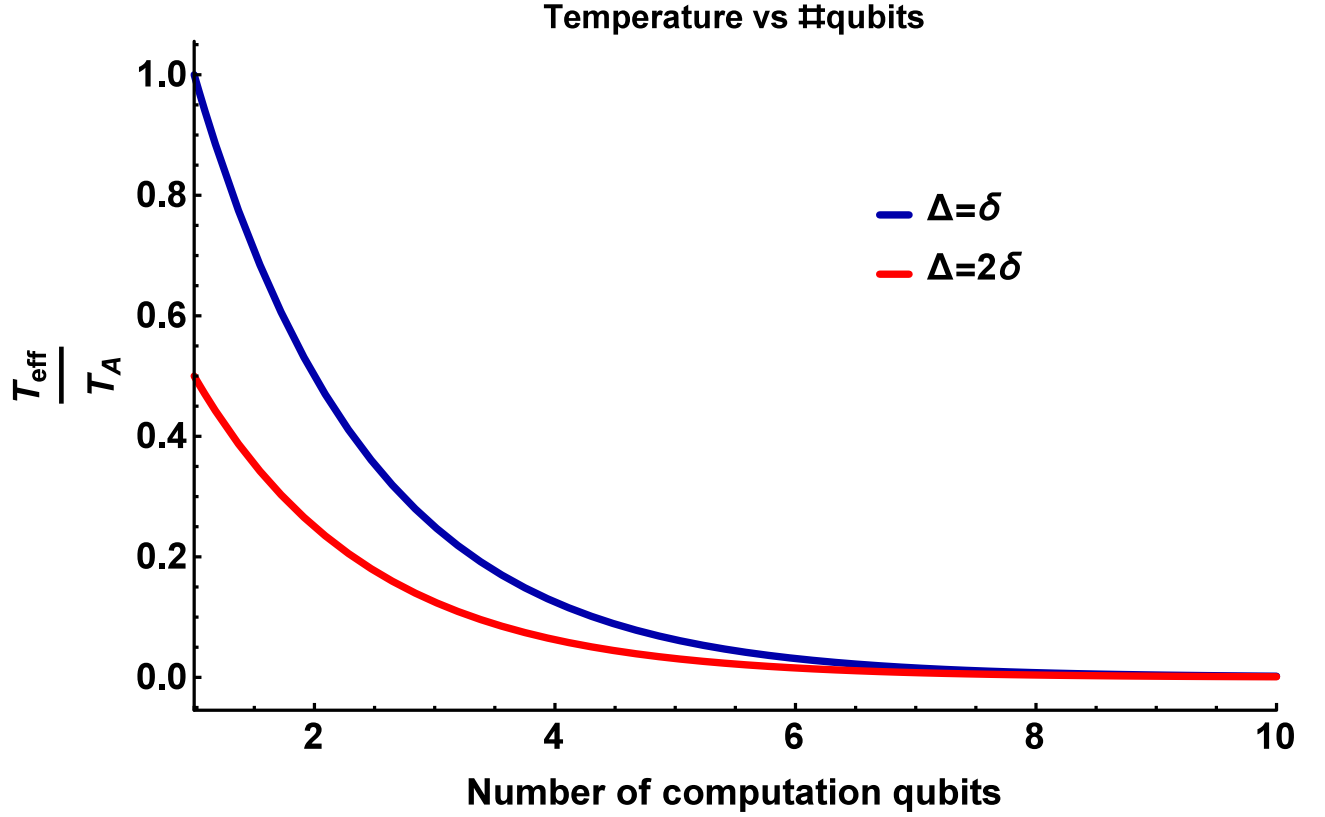


Figure 4. Asymptotic cooling ratio. The cooling limit depends on the number of qubits and the ratio of the energy gaps of the computation qubit to the one for the reset qubit, $\frac{\delta}{\Delta}$. The cooling limit improves exponentially with increasing n and linearly with decreasing $\frac{\delta}{\Delta}$.

It is interesting that despite the more complicated energy structure of the reset qubit, the “large gap” is the only parameter that would influence the cooling limit. In particular, the cooling limit does not directly depend on the number of energy levels or the spacing between them, as long as the total gap does not change.

This result also implies that a multi-qubit reset is linearly better than a single qubit reset. The energy gap of a multi-qubit reset system is the sum of the energy gaps of the individual qubits and as a result it has a larger gap which would improve the cooling limit. For instance, if k identical qubits are used for the reset, then the energy gap would be $\Delta_{total} = k \Delta$ and it lowers the cooling limit by a factor of $\frac{1}{k}$.

Note that the energy structure of the reset system could still change the complexity or the number of operations for HBAC but the asymptotic state only depends on the largest gap of the reset system.

In conclusion, we establish the fundamental limit of cooling for all HBAC techniques and show that it reduces exponentially with the number of qubits. It also depends on the ratio of the energy gap of the reset qubit to the gap of the computation qubits. We studied the effects of the changes to the energy spectrum of the reset system and showed that only the large gap of the reset system affects the asymptotic state. In particular, the number of energy levels, for a constant energy gap, does not influence the cooling limit.

Note that experimental imperfections could affect the minimum achievable cooling. The HBAC operations are optimized based on the probability distribution at each step, and thus unknown errors in the probability distribution mean the cooling steps will not be optimal. It is therefore critical to investigate these imperfections. Some of these, like decoherence has been recently studied [32].

Besides the fundamental significance, the cooling limit could have practical applications as well. For instance, it could give a quantitative measure of imperfection for implementing and studying the HBAC. One natural choice would be the distance from the asymptotic state, ρ^∞ , which requires the full density matrix. This may be expensive experimentally. An easier solution is $|p_0 - p_0^\infty|$ which approaches zero as the state approaches the asymptotic cooling limit. Or, simply $|P_0 - 2^{n-1}\epsilon|$, where P_0 is the achieved polarization of the first computation qubit.

For experimental implementation of HBAC, this measure quantifies how far the experiment is from the cooling limit and gives a metric for the assessment of the progress in the experiment.

Similarly, it can be used for theoretical cost analysis of HBAC which requires a notion of distance from the asymptotic state. The number of operations that are needed to achieve a certain fidelity to the asymptotic state can be calculated in terms of such a distance. Some studies have investigated this problem in terms of the number of iterations required [24, 31, 33]. By calculating the cost of an iteration in terms of resources such as gates or time, one could build on these works in order to calculate the resource cost of implementing HBAC.

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I. PROOF OF THE ASYMPTOTIC STATE OF PPA AC

We first prove the Theorem 1 in the paper and its extension for qudit reset and then prove the convergence of the PPA algorithmic cooling.

Before we get to the proof, it is useful to explain a few details about the dynamics and the update rules of the PPA. We start by explaining “crossings” which are the building block of the cooling in PPA.

Crossings

When the reset qubit is reset, the ordering of the elements on the diagonal of the density matrix changes. These changes are what lead to the cooling. The reset step takes the state $[\rho] = \{\lambda_1, \lambda_2, \dots, \lambda_{2^{n+1}}\}$ of n computation qubits and one reset qubit to

$$[\rho'] = \{p_0, p_1, \dots, p_{2^n-1}\} \otimes [\rho_R],$$

where $p_i = \lambda_{2i+1} + \lambda_{2i+2}$ and $[\rho_R] = \{e^\epsilon, e^{-\epsilon}\}$. This can be generalized for the reset with a qudit $[\rho_R] = \{a_1, a_2, \dots, a_k\}$ as well. Although the probabilities p_i are sorted, the full density matrix is not necessarily sorted. For instance, for some indices $i < j$, and $m_i > m_j$, we could have

$$p_i a_{m_i} < p_j a_{m_j}, \quad (S1)$$

or similarly for some indices $i > j$, and $m_i < m_j$, we could get

$$p_i a_{m_i} > p_j a_{m_j}. \quad (S2)$$

In these cases, the sort operation in PPA would rearrange these terms and update the value of p_i . We refer to the conditions in equation (S1) and equation (S2) as “crossing from below” and “crossing from above” respectively.

Despite the complexity of different crossings, we can make the following general remarks.

Remark 2. Crossing from above If p_i combined with the reset qudit probabilities gives the values $\{p_i a_1, p_i a_2, \dots, p_i a_k\}$ and there is crossing from above (and none from below), the sort operation on all $k2^n$ probabilities yields the values $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_k = p_i a_k$ for the $(ik+1)$ th, $(ik+2)$ th, \dots $(ik+k)$ th probabilities (i.e. the probabilities that will add up to determine p'_i) such that

$$p_i a_j \geq \lambda_j \geq p_i a_k. \quad (S3)$$

Proof. The second inequality is easier to see. It comes from the fact that $\forall j < i, p_j \geq p_i$ and therefore, for any m , we have $p_j a_m \geq p_i a_k$.

The first inequality comes from the ordering. The value λ_j is by definition the first element that is $\geq \lambda_{j+1}$. One can use induction (starting with $k = j+1$ as the base case) to prove the first inequality. Specifically, if $\lambda_{j+1} \leq p_i a_{j+1}$ then (since $a_j \geq a_{j+1}$) we have $p_i a_j \geq \lambda_{j+1}$ implies which implies that $\lambda_j \leq p_i a_j$. \square

Remark 3. Crossing from below If p_{i+1} combined with the reset qudit probabilities gives the values $\{p_{i+1} a_1, p_{i+1} a_2, \dots, p_{i+1} a_k\}$ and there is crossing from below (and none from above), the sort operation on all $k2^n$ probabilities yields the values $\delta_1 = p_{i+1} a_1 \geq \delta_2 \geq \dots \geq \delta_k$ for the $((i+1)k+1)$ th, $((i+1)k+2)$ th, \dots $((i+1)k+k)$ th probabilities such that

$$p_{i+1} a_j \leq \delta_j \leq p_{i+1} a_1. \quad (S4)$$

The proof is similar to the one for crossing from above.

For simplicity we define a distance. Consider two consecutive elements of the density matrix, p_i and p_{i+1} . We define the following distance between the elements of the density matrix

$$d_i \stackrel{\text{Def}}{=} \log \frac{p_i}{p_{i+1}}. \quad (S5)$$

We use the distance and generalise the Theorem 1 in the following way.

Theorem 4. For PPA algorithmic cooling with a reset qudit $[\rho_R] = \{a_1, a_2, \dots, a_k\}$ where a_l are sorted decreasing and sum to 1 and for any iteration t , $d_i^t \leq \max \left\{ d_i^0, \log \frac{a_1}{a_k} \right\}$.

Proof. We focus on d_i for some arbitrary iteration and prove the bound.

After the reset step of the iteration, we break down the sort operation into two steps. First we separately sort the values $p_j a_l$ for $j \geq i+1$, and also the values $p_j a_l$ for $j \leq i$. This means that the sort does not involve sorting between terms of the form $p_i a_l$ and $p_{j \geq i+1} a_l$ nor between terms of the form $p_{i+1} a_l$ and $p_{j \leq i} a_l$.

Let λ_j be the $(k-j+1)$ th smallest number after the sort operation among the $p_j a_l$ values for $j \leq i$ and let δ_j be the j th largest value after the sort operation among the $p_j a_l$ values for $j \geq i+1$. Note that $\delta_1 = p_{i+1} a_1$ and $\lambda_k = p_i a_k$. In the next step we complete the sort by combining and sorting the probabilities that lie between $p_{i+1} a_1$ and $p_i a_k$.

Let's first consider the case that $\lambda_1 \geq \delta_1$ and $\lambda_k \geq \delta_k$. Then when we merge and resort the λ_j and δ_j values, for some integer $r \geq 0$ the values $\delta_1, \delta_2, \dots, \delta_r$ will appear among the largest k values, and $\delta_{r+1}, \dots, \delta_k$ will appear among the smallest k values. Similarly, the values $\lambda_1, \dots, \lambda_{k-r}$ will appear among the largest k values, and the values $\lambda_{k-r+1}, \dots, \lambda_k$ will appear among the smallest k values.

The sub-case where $r = 0$ corresponds to when there is no crossing between p_i and p_{i+1} (i.e. $p_i a_k \geq p_{i+1} a_1$) and we will come back to this case as well.

Let us next consider the sub-case that $1 \leq r \leq k/2$. Thus we get

$$\begin{aligned} p'_i &= \sum_{j=1}^r (\lambda_j + \delta_j) + \sum_{j=r+1}^{k-r} \lambda_j \\ p'_{i+1} &= \sum_{j=k-r+1}^k (\lambda_j + \delta_j) + \sum_{j=r+1}^{k-r} \delta_j. \end{aligned}$$

Using Remark 2 and Remark 3 we find the following bounds

$$\begin{aligned} p'_i &\leq \sum_{j=1}^r (p_i a_j + p_{i+1} a_1) + \sum_{j=r+1}^{k-r} p_i a_j \leq r a_1 (p_i + p_{i+1}) + p_i \chi \\ p'_{i+1} &\geq \sum_{j=k-r+1}^k (p_i a_k + p_{i+1} a_j) + \sum_{j=r+1}^{k-r} p_{i+1} a_j \geq r a_k (p_i + p_{i+1}) + p_{i+1} \chi, \end{aligned}$$

where $\chi = \sum_{j=r+1}^{k-r} a_j$. We want to show that $\frac{p'_i}{p'_{i+1}} \leq \frac{a_1}{a_k}$ which follows from the fact that $p_i a_k \leq p_{i+1} a_1$ when there is at least one crossing between p_i and p_{i+1} . In other words,

$$\frac{p'_i}{p'_{i+1}} \leq \frac{r a_1 (p_i + p_{i+1}) + p_i \chi}{r a_k (p_i + p_{i+1}) + p_{i+1} \chi} \leq \frac{r a_1 (p_i + p_{i+1})}{r a_k (p_i + p_{i+1})} \leq \frac{a_1}{a_k}.$$

Let us next consider the sub-case that $k/2 < r < k$. Thus we get

$$\begin{aligned} \Rightarrow p'_i &= \sum_{j=1}^{k-r} (\lambda_j + \delta_j) + \sum_{j=k-r+1}^r \delta_j \\ \Rightarrow p'_{i+1} &= \sum_{j=r+1}^k (\lambda_j + \delta_j) + \sum_{j=k-r+1}^r \lambda_j. \end{aligned}$$

Using Remark 2 and Remark 3 we find the following bounds

$$\begin{aligned} p'_i &\leq (k-r)(p_i + p_{i+1}) a_1 + (2r-k) p_{i+1} a_1 \\ p'_{i+1} &\geq (k-r)(p_i + p_{i+1}) a_k + (2r-k) p_i a_k \\ \Rightarrow p'_i / p'_{i+1} &\leq \frac{((k-r)(p_i + p_{i+1}) + (2r-k) p_{i+1}) a_1}{((k-r)(p_i + p_{i+1}) + (2r-k) p_i) a_k} \\ &\leq \frac{((k-r)(p_i + p_{i+1}) + (2r-k) p_{i+1}) a_1}{((k-r)(p_i + p_{i+1}) + (2r-k) p_{i+1}) a_k} \leq \frac{a_1}{a_k}. \end{aligned}$$

For the case where $r = 0$, we get

$$p'_i = \sum_{j=1}^k \lambda_j \leq \sum_{j=1}^k p_i a_j = p_i$$

$$p'_{i+1} = \sum_{j=1}^k \delta_j \geq \sum_{j=1}^k p_{i+1} a_j = p_{i+1}.$$

It follows that $\frac{p'_i}{p'_{i+1}} \leq \frac{p_i}{p_{i+1}}$.

Now we get to the case when either all the $\lambda_j \leq \delta_1 = p_{i+1} a_1$ or when all the $\delta_j \geq \lambda_k = p_i a_k$ (or both). If it is the former, we get $p'_i \leq k \delta_1 = k p_{i+1} a_1$ and we also know that $p'_{i+1} \geq k p_{i+1} a_k$ which gives the desired result. Similarly, if all the $\delta_j \geq \lambda_k$ then $p'_{i+1} \geq k p_i a_k$ and $p'_i \leq k p_i a_1$ which again leads to $p'_i/p'_{i+1} \leq a_1/a_k$.

So the distance d'_i is bounded above by $\max \left\{ d_i, \frac{a_1}{a_k} \right\}$ which proves the theorem. \square

Note that for the case of $k = 2$ and $a_1 = e^\epsilon$ and $a_2 = e^{-\epsilon}$ we get Theorem 1.

Now we use this to prove that all of the p_i converge.

To prove the convergence, we first prove that p_0 converges and then the convergence of all the p_i follows from that. In order to make the connection between the convergence of p_0 and other p_i , we use Theorem 4.

Theorem 5. *Let p_0^t be the first diagonal element of the reduced density matrix of the computation qubits in the t^{th} iteration of PPA algorithmic cooling. Then $\lim_{t \rightarrow \infty} p_0^t = p_0^\infty$, for some constant p_0^∞ .*

Proof. The sequence of values p_0^t are increasing because there can only be crossings from below for p_0 . The sequence is also upper-bounded, therefore it must converge: $p_0^\infty = \lim_{t \rightarrow \infty} p_0^t$. \square

Theorem 6. *Let p_i^t be the i^{th} diagonal element of the reduced density matrix of the computation qubits in the t^{th} iteration of PPA algorithmic cooling with a qubit reset $[\rho_R] = \frac{1}{e^{-\epsilon} + e^\epsilon} \{e^\epsilon, e^{-\epsilon}\}$. Then assuming that $d_i^0 \leq 2\epsilon, \forall i$, the limit $\lim_{t \rightarrow \infty} p_i^t = e^{-2i\epsilon} p_0^\infty$ exists. We refer to the limit as p_i^∞ .*

Proof. We already proved that the p_0^∞ exists. This means that

$$\lim_{t \rightarrow \infty} (p_0^{t+1} - p_0^t) = 0. \quad (\text{S6})$$

On the other hand, Theorem 4 implies that as $t \rightarrow \infty$

$$p_0^{t+1} - p_0^t = p_1^t \frac{e^\epsilon}{z} - p_0^t \frac{e^{-\epsilon}}{z}. \quad (\text{S7})$$

The limit of the last term, $p_0^t \frac{e^{-\epsilon}}{z}$ exists and the left hand side converges to zero, so $\lim_{j \rightarrow \infty} p_1^t$ must be $e^{-2\epsilon} p_0^\infty$. The convergence of the rest of the p_i^t follows by induction. Note that although there could be crossings from above for $i \geq 1$, the change from above approaches zero and we get

$$p_i^{t+1} - p_i^t = \zeta + p_{i+1}^t \frac{e^\epsilon}{z} - p_i^t \frac{e^{-\epsilon}}{z}, \quad (\text{S8})$$

where ζ accounts for the changes to p_i from crossings from above and $\lim_{t \rightarrow \infty} \zeta = 0$. Therefore we get

$$p_{i+1}^\infty = e^{-2\epsilon} p_i^\infty. \quad (\text{S9})$$

\square

For the PPA with a reset qudit $[\rho_R] = \{a_1, a_2, \dots, a_k\}$, the proof is similar. As $j \rightarrow \infty$ we get $(p_0^{t+1} - p_0^t) - (p_1^t a_1 - p_0^t a_k) \rightarrow 0$ and since as $t \rightarrow \infty$ the left hand side and the last term converge, so does p_1^t . The rest of the proof follows similarly.

If we start with a maximally mixed state for the computation qubits, $d_i^0 = 0$, i.e. initially all the distances are zero, then for any iteration t and any index i , we get

$$d_i^t \leq \log \left(\frac{a_1}{a_k} \right) \quad (\text{S10})$$

and thus Theorem 6 (and its generalization to qudits) applies.

Note that for the case where the qubits are not initially in the maximally mixed state, Theorem 4 still applies and can be used to find the asymptotic state. A sufficient condition for getting the asymptotic state in Equation (4) is that $\log_2(\frac{p_0^0}{p_{2^n-1}^0}) \leq 2(2^n - 1)\epsilon$.

For the more general case of $[\rho^0] = \{p_0^0, p_1^0, \dots, p_{2^n-1}^0\}$, it is more complicated to determine the asymptotic state, however, Theorem 4 applies. In this case, the probabilities could be grouped in different blocks of consecutive probabilities where in each block, the distance between any two consecutive p_i^0 is less than 2ϵ and is greater between two different blocks. Using the theorem, we can see that the distance between the probabilities in each block would increase to 2ϵ . This also implies that two neighbouring blocks may merge together. To find the asymptotic state, we can go through the expansion and merger of all the blocks until the final asymptotic state is found. The asymptotic state would be a combination of different blocks where $d_i^\infty = 2\epsilon$ inside the blocks and is greater than that between the blocks.